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Appendix A

Detecting Change as it Occurs

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Abstract

Traditionally climate changes have been detected from long series of observations and long after they have happened. Our "inverse sequential" procedure, for detecting change as soon as it occurs, describes the existing or most recent data by their frequency distribution. Its parameter(s) are estimated both from the existing set of observations and from the same set augmented by 1, 2, ...*j* new observations. Individual-value probability products ("likelihoods") are used to form ratios which yield two probabilities for erroneously accepting the existing parameter(s) as valid for the augmented data set, and vice versa. A genuine parameter change is signalled when these probabilties (or a more stable compound probability) show a progressive decrease. New parameter values can then be estimated from the new observations alone using standard statistical techniques.

The inverse sequential procedure will be illustrated for global annual mean temperatures (assumed normally distributed), and for annual numbers of North Atlantic hurricanes (assumed to represent Poisson distributions). The procedure has been developed, but not yet tested, for linear or exponential trends, and for chi-square means or degrees of freedom, a special measure of autocorrelation (Radok, 1992).

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Detecting change as it occurs

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I. Introduction

The detection of changes in a developing time series requires some idea of what form they are likely to take. When the nature of the forcing is known, filters can be designed that will show their effects most clearly (Kim and North, 1991), but that knowledge is often not available in the geophysical sciences. There are many time series which can be viewed as potentially inhomogeneous, made up of irregular-length sections each of which differs from its neighbors in one or more of the parameters that define its signal and noise characteristics. As long as its parameters remain unchanged, an individual section can then be said to be in "statistical control" (Shewhart, 1939).

There exists considerable evidence that this concept is realistic in many geophysical contexts, for instance those exhibiting the "Hurst phenomenon" much discussed in hydrology (e.g., Klemes, 1974). With its minimum of arbitrary assumptions, the concept of statistical control suggests a general monitoring approach that registers the length and end of each controlled state, together with the new parameter values. The magnitude of changes in geophysical parameters cannot be anticipated, but their surveillance might use a probability for regarding the parameters established from existing observations as significantly changed by the addition of one or more new observations.

Such a "sequential" use of accruing information was pioneered by Wald (1945) and has developed into a large special field of statistics (cf. e.g., Gosh, 1988) which includes a range of procedures utilizing cumulative sums ("cusum" techniques; e.g., Goel, 1982)). The typical outcome in the simplest situation is a decision, with prescribed error probabilities, to accept one of two specified parameter values, or to continue sampling.

The "inverse" sequential approach here presented instead progressively determines "no-change" probabilities for parameter estimates based, respectively, on the accrued data and on the same data augmented by one or several new observations. A parameter change is then signaled when these probabilities begin decreasing to small values.

The basic relations for such a procedure are developed in section 2 and formulated for the means and variances of Gaussian and Poisson variates in Appendix A; mathematical derivations can be found in a paper submitted for publication in the American Statistician, and in a project report in preparation which will include computer programs for performing the calculations. These are illustrated in section 3, and a well-known way of combining the probabilities for several parameters into a change "fingerprint" is recalled in the last section.

2. Theory

Consider a series of m observations x_i, $i = 1,2,...m$, to which further j observations are added ($j = 1,2,...$). For a parameter θ (such as mean, variance, trend, etc.) the first m values yield an optimum estimate θ_m which the additional j observations change to θ_{m+j}. Writing the corresponding probabilities of individual x as p_m and p_{m+j}, respectively, the likelihood function of the first m observations is $\prod_1^m p_m = L_m(m)$ when $\theta = \theta_m$, and $\prod_1^m p_{m+j} = L_{m+j}(m)$ when $\theta = \theta_{m+j}$.

Here the bracketed number indicates the number of observations in the product, while the subscript is the number of observations used for the parameter estimate. The likelihood ratio $q(m) = L_{m+j}(m) / L_m(m) < 1$ if θ_m represents an optimum estimate for the m observations. In the same way we define $L_{m+j}(m+j)$ and $L_m(m+j)$ for the $m+j$ observations which yield a likelihood ratio $q(m+j) = L_{m+j}(m+j) / L_m(m+j) > 1$. The likelihoods and their ratios provide the elements for a formal test of two hypotheses. The first, $H(m)$, states that $\theta = \theta_m$ for the existing m observations, while the second, $H(m+j)$, is $\theta = \theta_{m+j}$ for the augmented set of $m+j$ observations.

Integration of the likelihood function $L_m(m)$ over its m-dimensional sample space $R(m)$ gives the probability of accepting the hypotheses $H(m)$ when true as $1-\alpha$, where α is the probability that $H(m)$ will be rejected when the sample point falls into a remote "critical' rejection region of the sample space, even though $H(m)$ remains true there ("type I error"). The corresponding integration of $L_{m+j}(m)$ leads to a second probability, β, that $H(m+j)$ is erroneously rejected when the sample point falls in the same region; this is also the probability of accepting the hypothesis $H(m)$ when false ("type II error"). The integrated likelihood ratio for the m observations thus becomes

$$q^*(m) = \frac{\iiint\limits_{R(m)} \ldots L_{m+j}(m)\ \mathrm{d}x_1\ \mathrm{d}x_2 \ldots \mathrm{d}x_m}{\iiint\limits_{R(m)} \ldots L_m(m)\ \mathrm{d}x_1\ \mathrm{d}x_2 \ldots \mathrm{d}x_m} = \frac{\beta}{1-\alpha}. \tag{1}$$

Applying the same argument to the augmented set of m+j observations leads to

$$q^*(m+j) = \frac{\iiint\limits_{R(m+j)} \ldots L_{m+j}(m+j)\ \mathrm{d}x_1\ \mathrm{d}x_2 \ldots \mathrm{d}x_{m+j}}{\iiint\limits_{R(m+j)} \ldots L_{m+j}(m)\ \mathrm{d}x_1\ \mathrm{d}x_2 \ldots \mathrm{d}x_{m+j}} = \frac{1-\alpha'}{\beta'}. \tag{2}$$

Disregarding the slight difference between the critical regions of$R(m)$ and $R(m+j)$ for the two data sets, we can approximate α', the probability of rejecting $H(m+j)$, when true, by β, the probability of accepting $H(m)$ when false; on a similar argument, $\beta' \approx \alpha$, so that equation (2) takes the approximate form

$$q^*(m+j) \approx \frac{1-\beta}{\alpha} \tag{3}$$

For the inverse sequential procedure we replace the q^* by the observed sample values q of the likelihood ratios, and from (1) and (3) obtain two relations for estimating α and β:

$$\alpha = \frac{(1 - q_m)}{(q_{m+j} - q_m)} \tag{4a}$$

$$\beta = \frac{(q_{m+j}\, q_m - q_m)}{(q_{m+j} - q_m)}. \tag{4b}$$

Equations (1) and (3) state the familiar decision limits of Wald's (1945) sequential probability ratio test (SPRT). Our argument in effect places the likelihood ratio $q(m)$ on Wald's lower decision limit, and the ratio $q(m+j)$ on different upper decision limits. But in contrast to a SPRT, now those limits involve known likelihood ratios $q(m)$ and $q(m+j)$ and unknown probabilities α and β. A definite change of control, from θ_m to θ_{m+j}, is signalled when both probabilities decrease to small values.

In practice rounding errors can raise the likelihood ratio $q(m)$ to values larger than unity and similarly lower $q(m+j)$ to values below one. Equations (4) then give unrealistic probabilities that are negative or larger than 1. Such q values may be replaced by 1, giving the probabilities the values 0 and 1, respectively, (or 0.5 if both q are taken as 1).

For monitoring the average of the two error probabilities can be used, but a more robust single no-change probability is defined by the ratio $q(m+j)/q(m)$. We write

$$\frac{q(m+j)}{q(m)} = \frac{(1-\alpha)(1-\beta)}{\alpha\beta} = \left(\frac{(1-\gamma)}{\gamma}\right)^2 = Q\,. \tag{5}$$

Taking square roots and solving for γ leads to

$$\gamma = (1 + \sqrt{Q})^{-1}\,. \tag{6}$$

The probability γ remains between 0 and 1/2 for $q(m+j) > q(m)$, and can be shown to fall between the arithmetic and geometric means of the two probabilities defined by (4a) and (4b).

Inverse sequential formulae for $q(m)$ and $q(m+j)$ are given in appendix A. The next section illustrates their use for monitoring changes in Gaussian and Poisson means and variances.

3. Applications

The procedure developed in section 2, and explicitly formulated in appendix A, tests the "null hypothesis" that the originally available data in question remain homogeneous as new data are added. A developing inhomogeneity becomes apparent first as a progressive decrease in the "no-change" probability γ, but that decrease will only continue all the way to small values when the parameters for the augmented (original plus new) data differ significantly from those valid for the original data alone. Clearly parameter estimates derived solely from the new data will show such differences well before the augmented set can do so. Therefore, the inverse sequential test is terminated as soon as a systematic decrease in γ has been firmly established; standard statistical procedures can then be used to compare the parameters of the original data with those derived from the new data that caused the probability decrease. That final step is omitted in the examples that follow since its result in general must be assessed by geophysical considerations as well as by its statistical significance.

As a first application we attempt to detect changes of mean and variance in two series of global mean temperature anomalies (deviations from the long-term mean 1958-77) reported by Angell and Korshover (1987; updated in Boden et al., 1990). Figure 1a shows these data for the surface and Figure 2a for the upper troposphere/lower stratosphere (the layer between the 100 hPa and 300 hPa constant-pressure surfaces).

The three probabilities for the surface observations are given in Figure 1b; they suggest a change in control around 1980. The test is then continued with the new larger mean and variance based on the observations for the years 1979-83; no further control changes are evident from the remaining data.

The probabilities for the temperature anomalies of the upper troposphere/lower stratosphere are given in Figure 2b. No changes of control can be discerned, although the mean decreased slightly from its initial value towards the end of the period of record used.

A second application of the inverse sequential procedure uses the annual numbers of tropical hurricanes recorded for the North Atlantic by Case (1988; updated to 1990) as shown in Figure 3a. The frequency distribution of these numbers for the period 1931-1990 (Figure 4) broadly conforms to a Poisson distribution with a mean of 5.6 (dashed lines in Figure 4).

Figure 3b gives the three error probabilities. A weak change of control is suggested to have occurred around 1940, with a decrease in the mean number to 3.8, followed by a more distinct change to a mean number of 7.6 around 1950. A renewed decrease back to the original mean number of 5.6 hurricanes per year is suggested by the gradual decrease of γ in the early 1960s. The remaining data show no further changes of control, even when a new base period is adopted in the 1970s in order to sharpen the test.

4. Conclusion

The inverse sequential procedure here described represents a new approach to the monitoring of time series, and clearly requires further experimentation and development. Mathematical details have already been formulated for detecting changes in linear and exponential trends, and in the means of chi-square variates which also represent their degrees of freedom and can be used as a measure of autocorrelation (Radok, 1992). We plan to apply the full procedure to the geophysical data provided in CD-ROM format by NASA under the Greenhouse Effect Detection Experiment (GEDEX; Schiffer and Unimayar, 1992; Olsen and Warnock, 1992). Another data archive to be tested is the Comprehensive Ocean Atmosphere Data Set (COADS; Woodruff et al., 1987; Diaz and Brown, 1992).

As further steps in the procedure, the lengths of statistically controlled sections can themselves be analyzed as a potential Poisson variate, and the independent probabilities obtained for different variables can be combined following Fisher (1941, section 21.1) to construct "fingerprints " of climatic change in the form of chi-square variates with $2k$ degrees of freedom,

$$\chi^2_{2k\ \mathrm{d.f.}} = \sum_{i=1}^{k}(-2\log_e \gamma_i)\ , \tag{6}$$

where k is the number of independent probabilities combined.

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Figure captions

Figure 1. Inverse sequential test applied to global surface temperature anomalies.
a) Annual mean deviations °C from 1958-77 mean (Angell and Korshover, 1987; updated in Boden et al., 1990).
b) Probabilities that no parameter changes are occurring. For symbols see text.

Figure 2. Inverse sequential test applied to global temperatures of the upper troposphere/lower stratosphere (100-300 hPa layer).
a) Annual mean deviations °C from 1958-1977 mean (Angell and Korshover, 1987; updated in Boden et al., 1990).
b) Probabilities that no parameter changes are occurring. For symbols see text.

Figure 3. Inverse sequential test applied to hurricane numbers.
a) Annual number of North Atlantic hurricanes, 1931-1990 (Case, 1988; updated).
b) Probabilities that no change in the mean number is occurring. For symbols see text.

Figure 4. Frequency histograms of hurricane numbers (solid lines) and Poisson distribution with mean 5.6 (dashed lines).

Appendix A: Inverse sequential formulae for means and variances of random samples from Gaussian and Poisson distributions

The restrictions to these distributions imply a need to verify that the data are indeed so distributed, and to perform an appropriate transformation if they are not (as described by e.g. Curtiss, 1943). The formulae give the basic probability p in the likelihood functions for m and $m+j$ observations, and the likelihood ratios $q(m)$ and $q(m+j)$ used to calculate the probabilities α, β, and γ from equations (4) and (6) in section 2. Subscripts indicate the number of values used for parameter estimates, and bracketed symbols give the numbers used to calculate the likelihoods and their ratios.

(1) Gaussian mean and variance

The basic probability,

$$p = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-(x-\mu)^2}{2\sigma^2}\right], \qquad \text{(A1)}$$

involves two parameters which cannot be separated in the test since in the present context neither parameter is prescribed. As an estimate for the distribution mean μ we use the sample mean $\bar{x}_n$; the distribution variance is estimated as $\sigma_n^2 = [n/(n-1)]s_n^2$, where s_n^2 is the sample variance and n (=m or $m+j$) the number of values used for the estimates. Then the two likelihood ratios are given by

$$q(m) = \exp\left[m \log_e \frac{\sigma_m}{\sigma_{m+j}} + \frac{m-1}{2}\left(1 - \frac{\sigma_m^2}{\sigma_{m+j}^2}\right) - \frac{m}{2\sigma_{m+j}^2}(\mu_{m+j} - \mu_m)^2\right], \qquad \text{(A2)}$$

and

$$q(m+j) = \exp\left[(m+j) \log_e \frac{\sigma_m}{\sigma_{m+j}} + \frac{m+j-1}{2}\left(\frac{\sigma_{m+j}^2}{\sigma_m^2} - 1\right) + \frac{(m+j)(\mu_{m+j} - \mu_m)^2}{2\sigma_m^2}\right]. \qquad \text{(A3)}$$

(2) Poisson mean (=variance)

This case is simpler because the basic probability,

$$p = \frac{\bar{x}^x}{x!\,\exp(\bar{x})}, \qquad \text{(A4)}$$

has only a single parameter $\bar{x}$, the mean number of occurrences. The likelihood ratios are

$$q(m) = \exp\left[m\left\{\bar{x}_m \log_e \frac{\bar{x}_{m+j}}{\bar{x}_m} - (\bar{x}_{m+j} - \bar{x}_m)\right\}\right], \qquad \text{(A5)}$$

and

$$q(m+j) = \exp\left[m+j \left\{ \bar{x}_{m+j} \log_e \frac{\bar{x}_{m+j}}{\bar{x}_m} - (\bar{x}_{m+j} - \bar{x}_m) \right\} \right]. \tag{A6}$$

References

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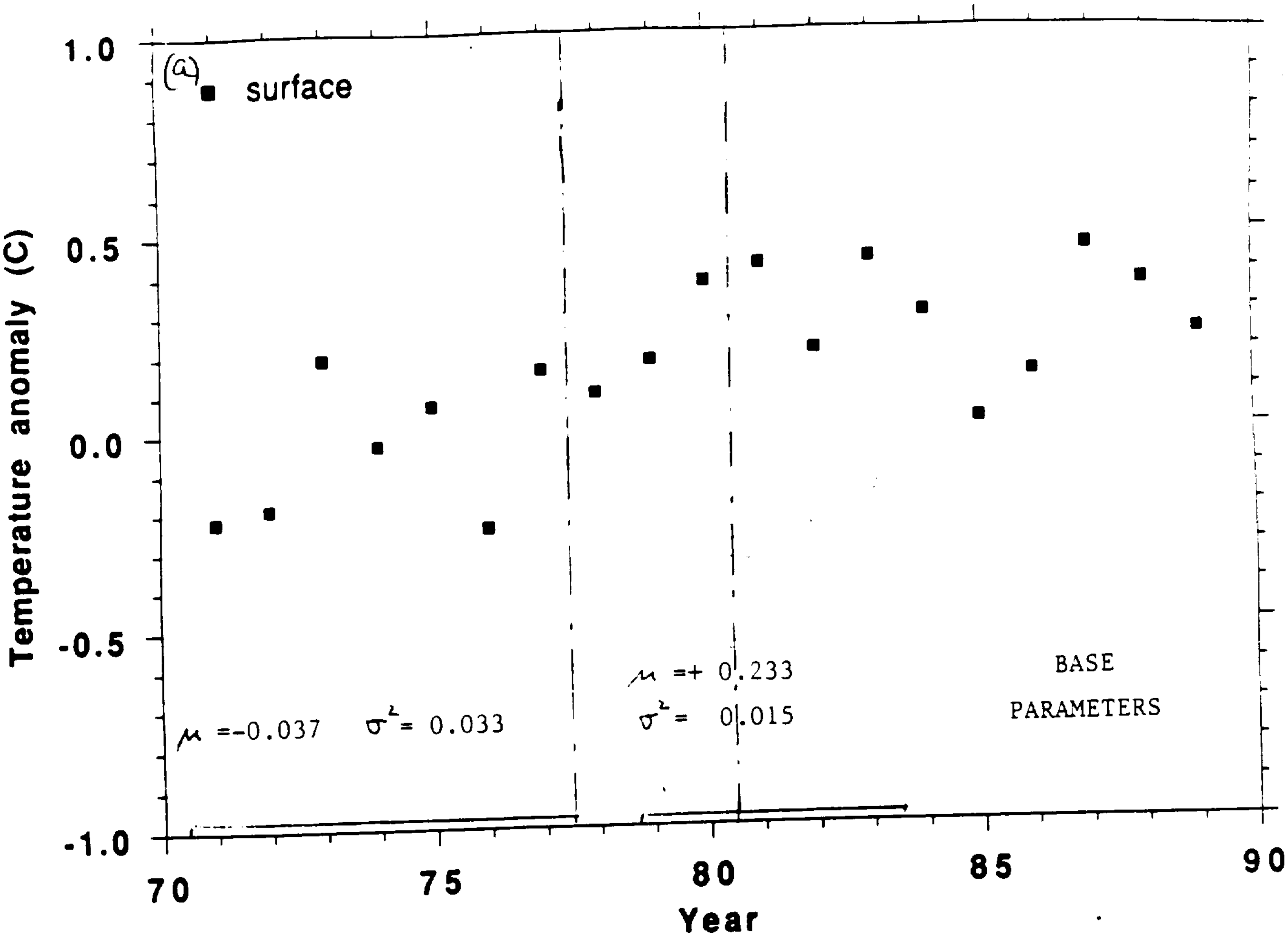
GLOBAL ANNUAL MEAN TEMPERATURE ANOMALIES FROM 1958-77 MEAN (ANGELL&KORSHOVER 1987)



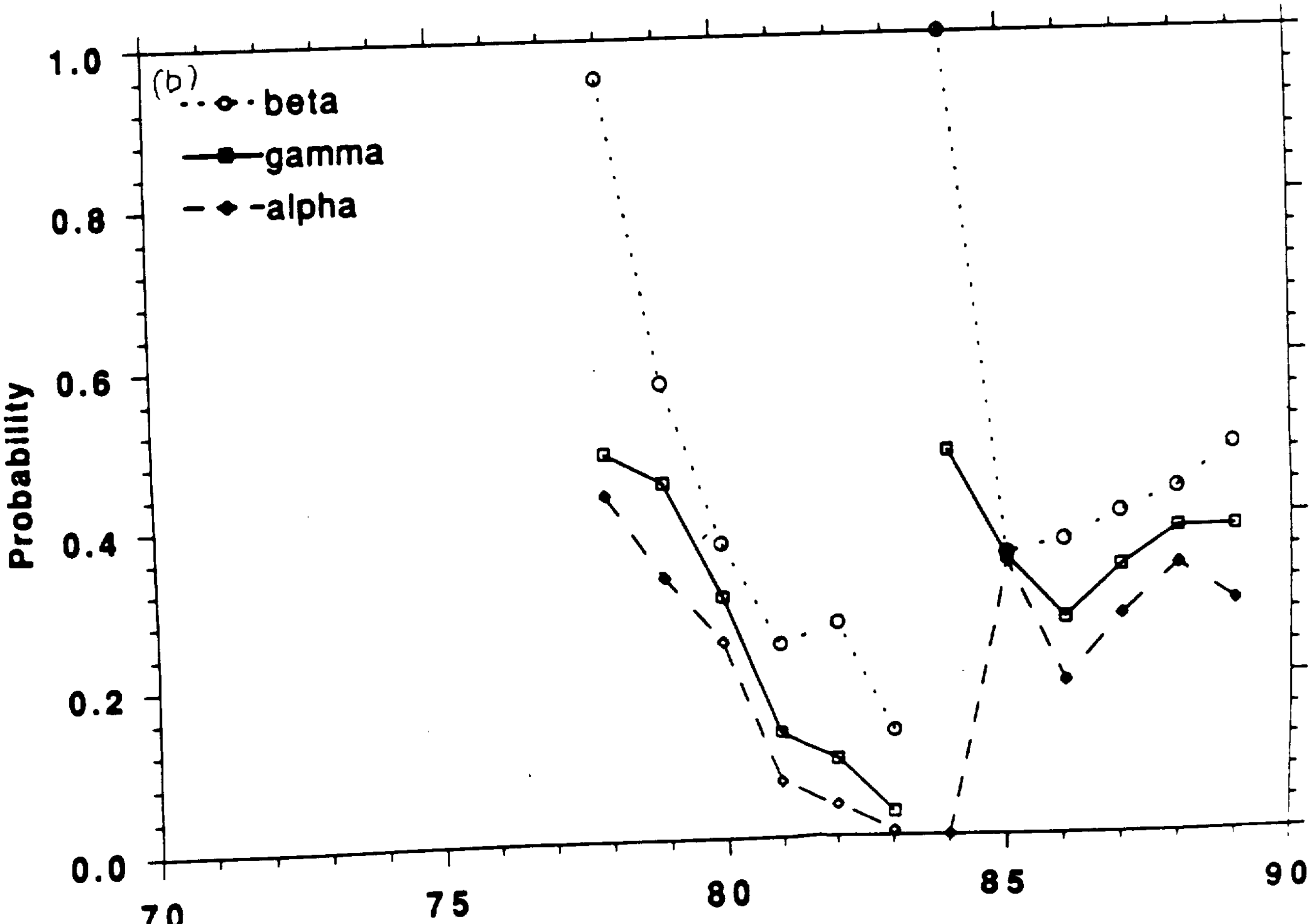
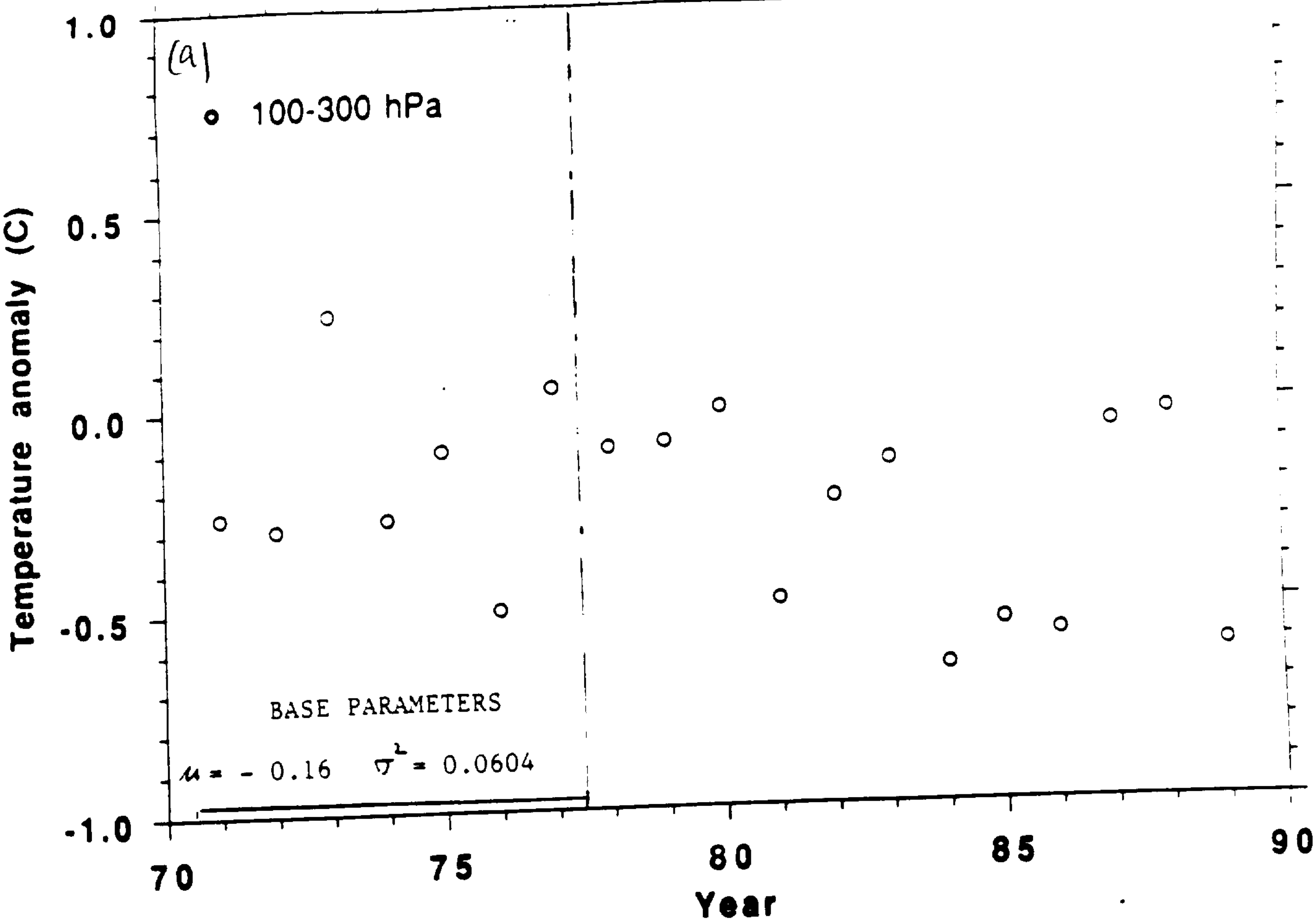


Fig. 1

GLOBAL ANNUAL MEAN TEMPERATURE ANOMALIES FROM 1958-77 MEAN (ANGELL & KORSHOVER 1987)



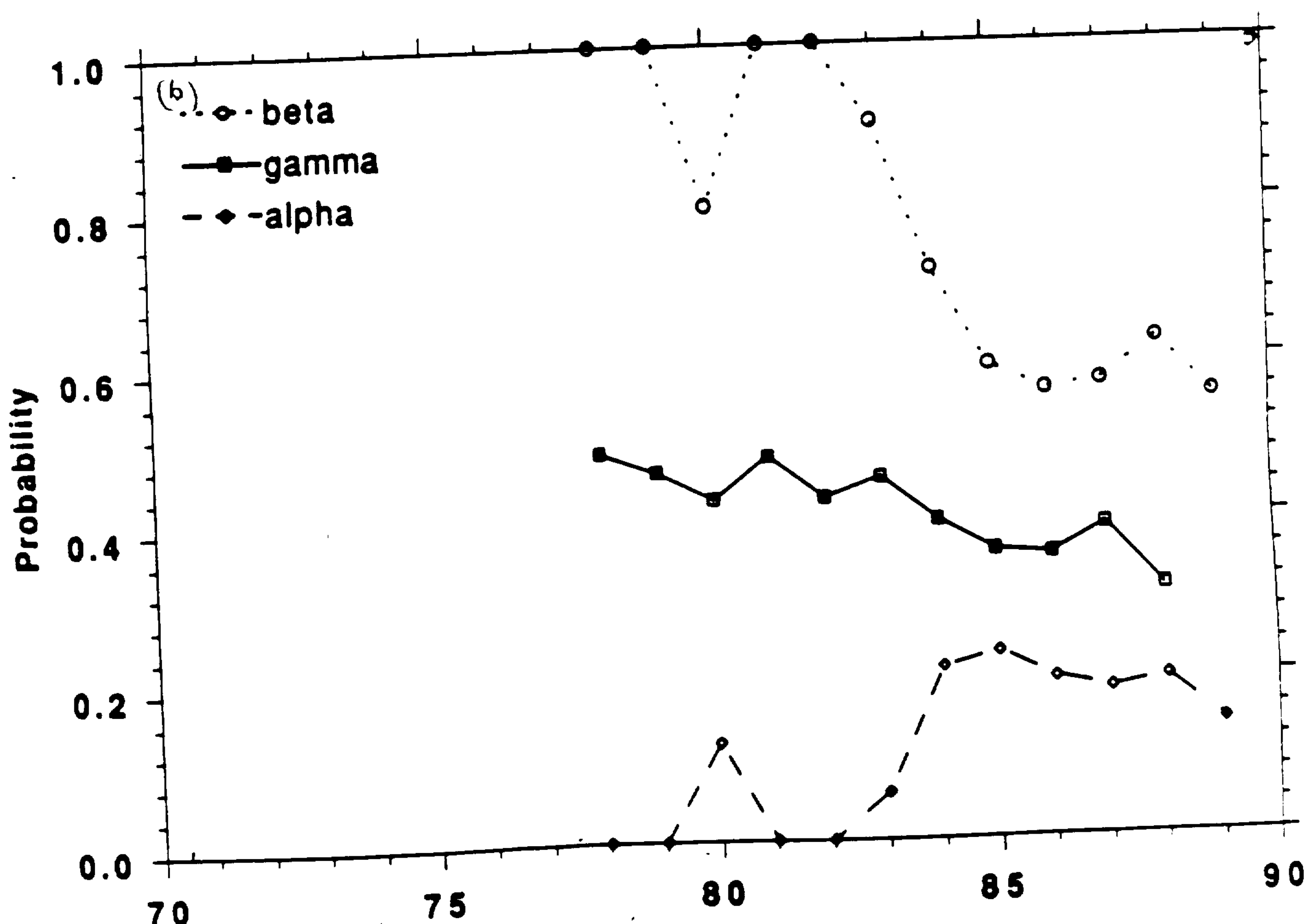


fig. 2

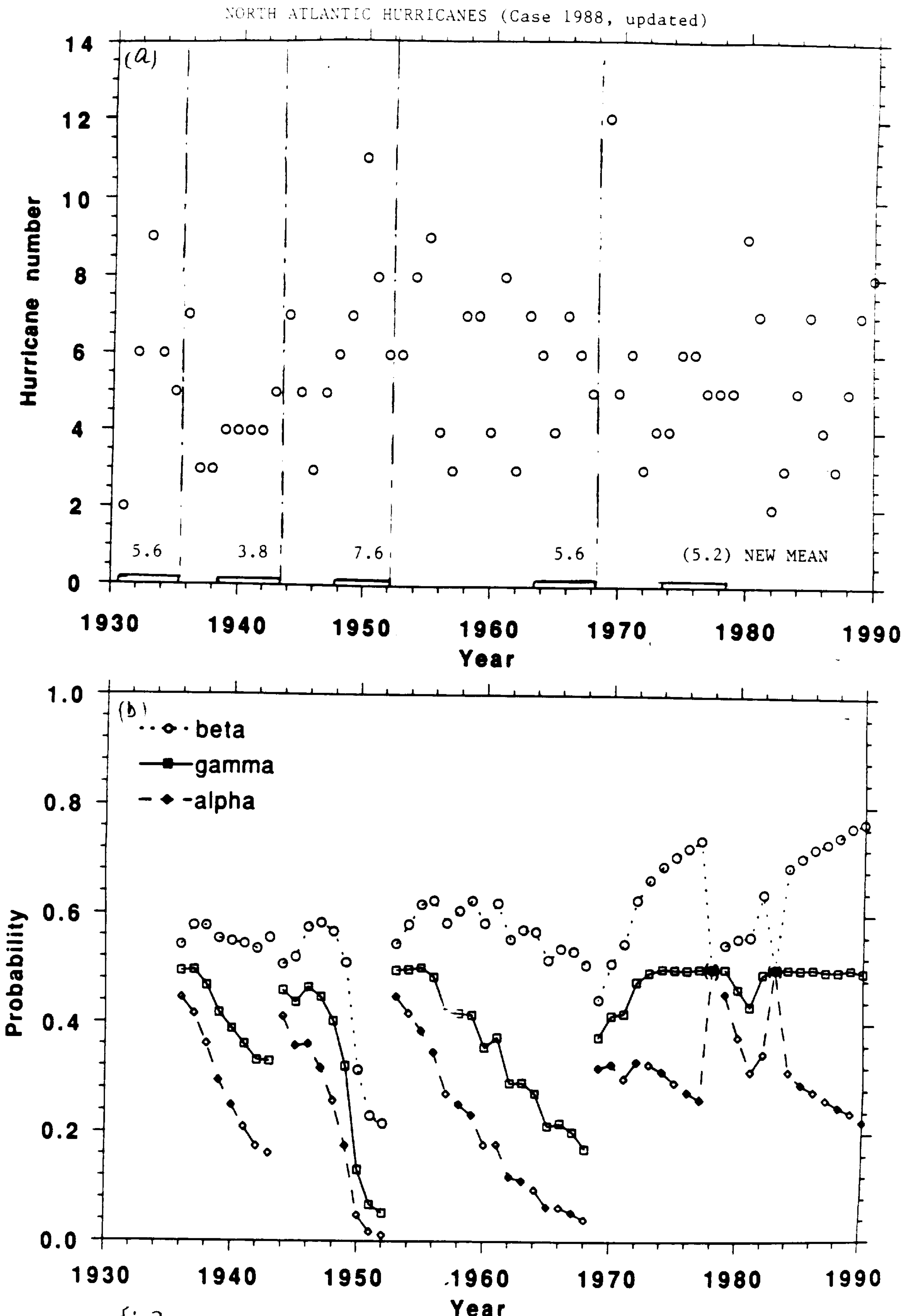
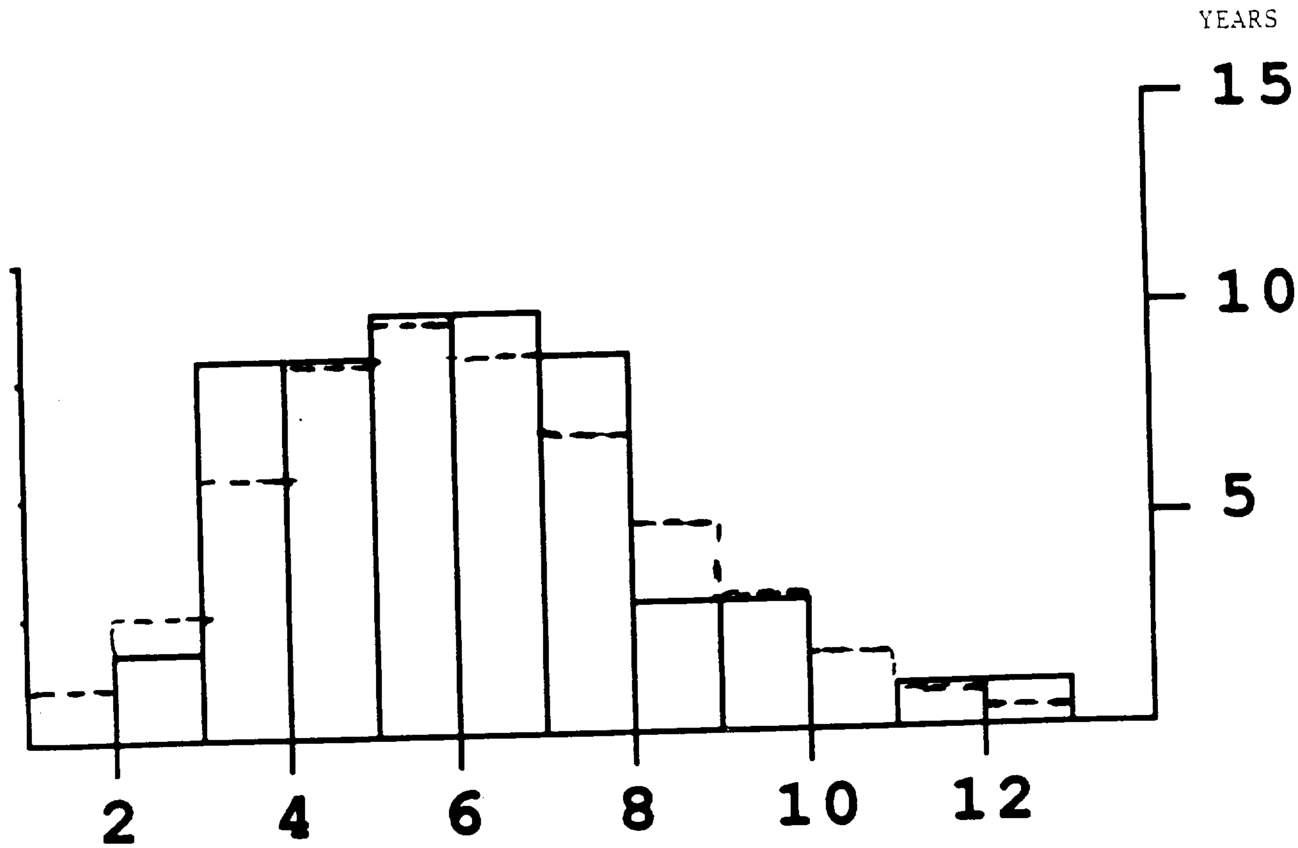

NORTH ATLANTIC HURRICANES (Case 1988, updated)
(a)
Hurricane number
5.6
3.8
7.6
5.6
(5.2) NEW MEAN
Year
(b)
beta
gamma
alpha
Probability
Year

fig.3



ANNUAL NUMBER OF NORTH ATLANTIC HURRICANES (CASE 1987,update)

----- POISSON DISTRIBUTION WITH MEAN 5.6

fig.4